

Pentanedioic acid, 3,3-dimethyl-
4839-46-7 | DTXSID9063617

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 7.79e-01

Global applicability domain: Inside

Local applicability domain index: 6.33e-01

Confidence level: 8.49e-01

Nearest Neighbors from the Training Set

| | | |
|--|---|---|
| <div>Image not found</div> <div>2,2-Dimethylpentanedioic acid</div> <div>Measured: 0.67</div> <div>Predicted: 7.43e-01</div> | <div>Image not found</div> <div>Heptanedioic acid</div> <div>Measured: 0.61</div> <div>Predicted: 6.46e-01</div> | <div>Image not found</div> <div>4-oxo-2-propylpentanoic acid</div> <div>Measured: 1.31</div> <div>Predicted: 1.27</div> |
| <div>Image not found</div> <div>Hexanedioic acid</div> <div>Measured: 0.08</div> <div>Predicted: 6.25e-02</div> | <div>Image not found</div> <div>2,2-Dimethylpropanoic acid</div> <div>Measured: 1.48</div> <div>Predicted: 1.48</div> | |